

Scaling and Enhanced Symmetry at the Quantum Critical Point of the Sub-Ohmic Bose-Fermi Kondo Model

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We consider the finite temperature scaling properties of a Kondo-destroying quantum critical point in the Ising-anisotropic Bose-Fermi Kondo model (BFKM). A cluster-updating Monte Carlo approach is used, in order to reliably access a wide temperature range. The scaling function for the two-point spin correlator is found to have the form dictated by a boundary conformal field theory, even though the underlying Hamiltonian lacks conformal invariance. Similar conclusions are reached for all multi-point correlators of the spin-isotropic BFKM in a dynamical large- N limit. Our results suggest that the quantum critical local properties of the sub-ohmic BFKM are those of an underlying boundary conformal field theory.

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Quantum criticality is currently being discussed in the contexts of a wide array of strongly correlated electron systems. A prototype is provided by a family of heavy fermion metals near their antiferromagnetic quantum critical point (QCP). The physical properties of these materials drastically deviate from the expectations of the traditional theory of quantum criticality[1, 2, 3, 4], so much so that the question has been raised as to whether and how the Kondo effect itself becomes critical at the antiferromagnetic quantum transition[5, 6, 7]. Through the extended dynamical mean field theory, the self-consistent BFKM provides one means to elucidate such Kondo-destroying quantum criticality[5]. The sub-Ohmic BFKM is also the appropriate low-energy model for single-electron transistors attached to ferromagnetic leads[8]. One clue[9, 10, 11] about the nature of the quantum criticality in the sub-Ohmic BFKM is the failure of the standard description[12] in terms of fluctuations of the classical order parameter in elevated dimensions. Nonetheless, a proper field theory for the QCP is not yet available. To address this pressing open issue, it is important to identify the symmetry of the QCP.

In this letter, we study the finite temperature scaling properties of the BFKM in some detail. We have been motivated by general considerations of a boundary conformal field theory[13, 14]. The latter arises in many quantum impurity problems whose bulk system in the continuum limit is conformally invariant. At zero temperature, the s-wave component of the bulk degrees of freedom can be thought of as living on a half-plane, which is composed of the imaginary time (τ) dimension and the radial spatial (r) dimension; the quantum impurity is located at the boundary of the half-plane[13]. At finite temperature (T), the extent along the imaginary time direction becomes finite, of length $\beta = 1/T$, and periodic boundary condition (along τ) turns it into a half-cylinder of circumference β . A conformal mapping between the half-plane and the half-cylinder[13, 15], say $z = \tan(\pi w/\beta)$, can then be used to obtain finite-temperature correlators from their zero-

temperature counterparts. The result is the well known scaling form[15, 16]

$$\langle \Phi(\tau, T) \Phi(0, T) \rangle = C \left(\frac{\pi/\beta}{\sin(\pi\tau/\beta)} \right)^{2\Delta}, \quad (1)$$

where Δ is the scaling dimension of Φ , a conformal primary field, and C a constant.

We present results here which show that the scaling functions of the two-point spin correlators of the sub-Ohmic BFKM have the form dictated by Eq. (1). Similar conclusions are drawn for multi-spin correlators of the model in a large- N limit. These results are surprising, since the sub-Ohmic nature [Eq. (3), with $\epsilon > 0$] of the bosonic spectrum implies that the bulk component of the Hamiltonian itself lacks conformal invariance. The results imply that the symmetry is enhanced at the boundary QCP of the BFKM, in such a way that the local properties are those of an underlying boundary conformal field theory (CFT).

Our focus will be the Ising-anisotropic spin-1/2 BFKM. In order to address the finite temperature scaling properties, it is important to access a wide temperature range with sufficiently high accuracy. Here, we develop a cluster-updating Monte Carlo method, and show that it can reliably reach temperatures as low as $10^{-4} T_K^0$, where T_K^0 is the Kondo scale of the fermion-only Kondo problem. The wide temperature range covered distinguishes this method from existing ones for Kondo-type systems[17, 18, 19].

BFKM with Ising Anisotropy: In a BFKM, a quantum spin is simultaneously coupled to a fermionic bath and a bosonic one. For the Ising-anisotropic case, the Hamiltonian is

$$\begin{aligned} \mathcal{H}_{\text{bfkm}} = & J_K \mathbf{S} \cdot \mathbf{s}_c + \sum_{p\sigma} E_p c_{p\sigma}^\dagger c_{p\sigma} \\ & + \tilde{g} \sum_p S^z \left(\phi_p + \phi_{-p}^\dagger \right) + \sum_p w_p \phi_p^\dagger \phi_p, \end{aligned} \quad (2)$$

where \mathbf{S} is a spin-1/2 local moment, $c_{p\sigma}^\dagger$ describes a fermionic bath with a constant density of states,

$\sum_p \delta(\omega - E_p) = N_0$, and ϕ_p^\dagger a bosonic bath whose spectrum is sub-Ohmic ($\epsilon > 0$):

$$\sum_p [\delta(\omega - \omega_p) - \delta(\omega + \omega_p)] \sim |\omega|^{1-\epsilon} \text{sgn}(\omega). \quad (3)$$

We adopt bosonization and a canonical transformation[19] to map $\mathcal{H}_{\text{bfkm}}$ to

$$\begin{aligned} \mathcal{H}'_{\text{bfkm}} = & \Gamma S^x + \Gamma_z S^z s_c^z + \mathcal{H}_0 \\ & + \tilde{g} \sum_p S^z (\phi_p + \phi_{-p}^\dagger) + \sum_p w_p \phi_p^\dagger \phi_p, \end{aligned} \quad (4)$$

where \mathcal{H}_0 and s_c^z describe the (bosonized) fermionic bath and local conduction electron spin. The quantities Γ and Γ_z are, respectively, determined by the spin-flip and longitudinal components of the Kondo coupling. Integrating out both the fermionic and bosonic baths, we arrive at the partition function $Z'_{\text{bfkm}} \sim \text{Tr} \exp[-S'_{\text{imp}}]$ with

$$\begin{aligned} S'_{\text{imp}} = & \int_0^\beta d\tau [\Gamma S^x(\tau) - \frac{1}{2} \int_0^\beta d\tau' S^z(\tau) S^z(\tau')] \\ & \times (\chi_0^{-1}(\tau - \tau') - \mathcal{K}_c(\tau - \tau')), \end{aligned} \quad (5)$$

where the trace is taken over spin degrees of freedom. $\chi_0^{-1} = \tilde{g}^2 \sum_p G_{\phi,0}$, and $\mathcal{K}_c(i\omega_n) = \kappa_c |\omega_n|$ ($\kappa_c \sim \Gamma_z^2 N_0^2$) came from integrating out the fermionic bath. Trotter decomposing the effective action and re-expressing the leading order (in $1/L$, L being the number of time slices) through the transfer matrix for a one-dimensional Ising model[20], one finally obtains,

$$\mathcal{Z} \sim \text{Tr} \exp \left[\sum_i K_{\text{NN}} S_i S_{i+1} + \sum_{i,j} K_{\text{LR}}(i-j) S_i S_j \right]. \quad (6)$$

The mapping procedure is essentially equivalent to what was done for the pure Kondo model[21]. The effective action at inverse temperature β is equivalent to that of a one-dimensional chain of L Ising spins, with a periodic boundary condition. The nearest neighbor interaction is $K_{\text{NN}} = -\ln(\tau_0 \Gamma/2)/2$, where $\tau_0 = \beta/L$; it is singular in the limit $\tau_0 \rightarrow 0$. $K_{\text{LR}}(i-j)$ is the sum of two ferromagnetic long-ranged interactions proportional to $1/|i-j|^2$ and $1/|i-j|^{2-\epsilon}$; it results from discretizing $(\chi_0^{-1}(\tau - \tau') - \mathcal{K}_c(\tau - \tau'))$:

$$K_{\text{LR}}(|i-j|) = \frac{\tau_0^2}{4} \left[\frac{2\alpha(\pi/\beta)^2}{\sin(\frac{\pi\tau_0|i-j|}{\beta})^2} + \frac{g(\pi/\tilde{\beta})^{2-\epsilon}}{\sin(\frac{\pi\tau_0|i-j|}{\tilde{\beta}})^{2-\epsilon}} \right]. \quad (7)$$

The coupling constant α is related to the electron scattering phase shift. We choose $\alpha = 1/2$, so that $g = 0$ corresponds to the Toulouse limit of the Kondo problem. For the most part, the parameter $\tilde{\beta} \gg \beta$ is taken to be $20000\tau_0$. (In the cases we have checked, we found identical results when the second term in the brackets is simply replaced by $g/\tau^{2-\epsilon}$.) The thermodynamic limit

has to be taken such that a finite T_K^0 is preserved, in order to have the temperature region of interest, $T < T_K^0$; in the limit $\tau_0 \rightarrow 0$ at finite β we approach the high-temperature fixed point. For the numerical values chosen in the manuscript we are always able to focus on the scaling properties in the low temperature range of $T \ll T_K^0$.

We study this model using a cluster-updating Monte Carlo (MC) scheme. The long-range nature of the interaction is most conveniently incorporated using the method of Ref. [22]. We specifically use a Wolff algorithm[23]. The improved estimator for the spin-spin correlation function implies that the susceptibility in Matsubara frequency is given by

$$\chi(i\omega_n) = \langle \left| \sum_{j \in \mathcal{C}} e^{i\omega_n \tau_j} \right|^2 / n_{\mathcal{C}} \rangle / TL, \quad (8)$$

where the sum runs over all spins in the cluster, $\langle \rangle$ indicates the average over all Monte Carlo runs and $n_{\mathcal{C}}$ is the number of spins in a given cluster. The susceptibility as a function of imaginary time τ is given by $\chi(\tau_n) = \frac{1}{4} \sum_{S_m^z, S_{m+n}^z \in \mathcal{C}} \langle S^z(\tau_m + \tau_n) S^z(\tau_m) \rangle$, where $\tau_n = n\tau_0$. We measure $\chi(i\omega_n)$ and $\chi(\tau_n)$ directly.

This method allows us to reach considerably lower temperatures than approaches using local updates[18, 19]. We typically build 2000 MC clusters as a warm-up and about $N_{\text{run}} = 10^6$ MC clusters at high temperatures and increase the number of clusters built to about 50000 warm-ups and about $N_{\text{run}} = 10^{10}$ clusters at $\beta = 512$ for all τ_0 . While every cluster built contributes to $\chi(\tau = 0)$ only the subset of clusters with spins separated by $\tau \geq \beta/2$ will contribute to $\chi(\tau \approx \beta/2)$. One might therefore expect that variance and autocorrelation effects strongly depend on τ , but this turned out not to be the case. For an error estimate, we performed a binning analysis of our data in order to obtain the integrated autocorrelation time τ_{int} and variance [30]. The relative error of our results is $(\Delta\chi)/\chi \approx 10^{-2}$ and below (depending on τ and β) and the integrated autocorrelation time is $\tau_{\text{int}} < 100 \ll N_{\text{run}}$ for all τ and β .

For concreteness, we will now present the results for $\epsilon = 0.4$.

Consider first the Kondo limit ($g = 0$). In Fig. 1(a) we show the static spin susceptibility versus temperature. It correctly captures the Pauli behavior at temperatures below T_K^0 . Because we have placed the Kondo couplings at the Toulouse point, we can compare our results with the exact expression: Fig. 1(a) demonstrates the agreement for more than 4 decades of temperature! In addition, our results for the dynamical susceptibility[24] are consistent with the standard expectations for the Kondo problem, including the asymptotic long time (low frequency) Fermi-liquid power-law behavior and the exact limit at short time, $\chi(\tau \rightarrow \tau_0) \rightarrow 1/4$.

Fig. 1(a) also shows the static susceptibility at the QCP, $g_c/T_K^0 = 0.821$. We find $\chi_{\text{stat}}(T, g_c) \sim 1/T^{0.608}$,

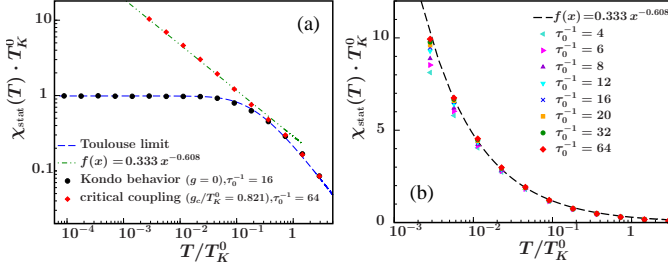


FIG. 1: (a) Static local spin susceptibility in the Kondo case ($g = 0$, $\tau_0 = 1/16$, black circles) and for the critical coupling ($\epsilon = 0.4, \Gamma = 0.75, g_c = 0.821T_K^0, \tau_0 = 1/64$, red diamonds). The dashed blue line is the fit to the Toulouse limit (see e.g. Ref. [29]), and the dashed dotted line a fit to the critical behavior. Defining $T_K^0 \equiv 1/\chi_{\text{stat}}(T=0)$ we obtain $T_K^0\tau_0 \approx 0.688$; (b) Static susceptibility at the critical coupling, for various values of the cutoff parameter, τ_0 .

for over two decades of temperature. Since $\chi(\omega, g_c) \sim 1/\omega^{1-\epsilon}$ is expected[25, 26], the temperature exponent is, within about 1% accuracy, the same as the frequency exponent; this is consistent with the NRG result[11]. The dependence of the critical susceptibility on the cutoff parameter τ_0 is illustrated in Fig. 1(b). Compared to the Kondo case (not shown), this dependence is stronger. However, within the measured temperature range, the result does not change significantly for the smallest three τ_0 values. We now turn to the τ -dependence of the dynamical spin susceptibility, $\chi(\tau, T)$, near the quantum critical coupling $g \approx g_c$. The scaling plot, Fig. 2, demonstrates that $\chi(\tau, T)$ is a function of $\pi T/\sin(\pi\tau T)$ only. In the long-time limit (lower-left corner), the dependence is a simple power-law for over two decades of $\pi T/\sin(\pi\tau T)$. We therefore reach one of our key results, namely

$$\chi_{\text{crit}}(\tau, T) = \Phi\left(\frac{\pi\tau_0 T}{\sin(\pi\tau T)}\right) \xrightarrow{T \ll T_K^0} c \cdot \left(\frac{\pi\tau_0 T}{\sin(\pi\tau T)}\right)^\epsilon, \quad (9)$$

for $\tau^{-1} \ll T_K^0$; here c is a constant (≈ 0.89). In other words, in the long-time (low-energy) limit, the two-point spin correlator has precisely the form dictated by a boundary CFT, inspite of the lack of conformal invariance in the Hamiltonian. This scaling form implies ω/T -scaling.

We now turn to complementary results on the multi-point correlators, which are provided by the large- N limit of a spin-isotropic BFKM.

Spin-isotropic BFKM in a large- N limit: The limit is taken for the Hamiltonian of the $\text{SU}(N) \times \text{S}(M)$ BFKM,

$$\begin{aligned} \mathcal{H}_{\text{MBFK}} = & (J_K/N) \sum_{\alpha} \mathbf{S} \cdot \mathbf{s}_{\alpha} + \sum_{p, \alpha, \sigma} E_p c_{p\alpha\sigma}^{\dagger} c_{p\alpha\sigma} \\ & + (g/\sqrt{N}) \mathbf{S} \cdot \mathbf{\Phi} + \sum_p w_p \mathbf{\Phi}_p^{\dagger} \cdot \mathbf{\Phi}_p, \end{aligned} \quad (10)$$

where the spin and channel indices are $\sigma = 1, \dots, N$ and $\alpha = 1, \dots, M$, respectively, and $\mathbf{\Phi} \equiv \sum_p (\mathbf{\Phi}_p + \mathbf{\Phi}_{-p}^{\dagger})$

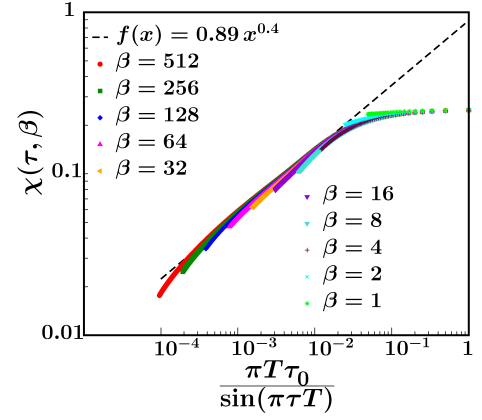


FIG. 2: Scaling of the local spin susceptibility (at the QCP), which is plotted as a function of $\pi T\tau_0/\sin(\pi\tau T)$. The parameters are $\epsilon = 0.4, \Gamma = 0.75, g = 0.821T_K^0 \approx g_c, \tau_0 = 1/64$. Note that $\pi T\tau_0/\sin(\pi\tau T)$ becomes small (order $\pi\tau_0/\beta$) as τ approaches the long-time limit, $\tau \rightarrow \beta/2$. The power-law collapse occurs over two decades of the parameter $\pi T\tau_0/\sin(\pi\tau T)$. The deviation at the low-left corner is attributed to finite-size effects.

contains $N^2 - 1$ components. This dynamical large- N limit[27, 28] is expressed in terms of pseudo-fermions f_{σ} and a bosonic decoupling field B_{α} , where $S_{\sigma, \sigma'} = f_{\sigma}^{\dagger} f_{\sigma'} - \delta_{\sigma, \sigma'} Q/N$, where Q is related to the chosen irreducible representation of $\text{SU}(N)$ [27]. The large- N equations are

$$\begin{aligned} \Sigma_B(\tau) &= -\mathcal{G}_0(\tau) G_f(-\tau); \\ \Sigma_f(\tau) &= \kappa \mathcal{G}_0(\tau) G_B(\tau) + g^2 G_f(\tau) \mathcal{G}_{\Phi}(\tau); \\ G_B^{-1}(i\omega_n) &= 1/J_K - \Sigma_B(i\omega_n); \\ G_f^{-1}(i\omega_n) &= i\omega_n - \lambda - \Sigma_f(i\omega_n); \end{aligned} \quad (11)$$

together with a constraint $G_f(\tau \rightarrow 0^-) = Q/N$. Here, $\kappa = M/N$, λ is a Lagrangian multiplier, $\mathcal{G}_0 = -\langle T_{\tau} c_{\sigma\alpha}(\tau) c_{\sigma\alpha}^{\dagger}(0) \rangle_0$, and $\mathcal{G}_{\Phi} = \langle T_{\tau} \Phi(\tau) \Phi^{\dagger}(0) \rangle_0$. Note that, when $g = 0$, the Kondo Hamiltonian contains a conformally-invariant bulk and the corresponding correlation functions naturally have the form of a boundary CFT[27, 28]. Here we address what happens at the QCP of the model with finite g [9], for which the bulk lacks conformal invariance.

Consider first the zero-temperature case. The quantum critical properties of the model have been determined in Ref. [9]. At $g = g_c$, both the pseudo-fermion propagator $G_f(\tau)$ and the auxiliary boson propagator $G_B(\tau)$ are critical; their leading terms are $G_f(\tau) = A/|\tau|^{\epsilon/2} \text{sgn}(\tau)$ and $G_B(\tau) = B/|\tau|^{1-\epsilon/2}$, respectively. Here, we observe that the local two-spin correlator, as well as all the local higher-multiple-spin correlators, factorize in terms of $G_f(\tau)$ according to Wick's theorem. This immediately implies that the scaling functions for all these correlators have the form of a boundary CFT. The dynamical spin susceptibility, e.g., is

$$\chi(\tau) \equiv \langle T_{\tau} S_{\sigma \neq \sigma'}(\tau) S_{\sigma' \sigma}(0) \rangle = -G_f(\tau) G_f(-\tau), \quad (12)$$

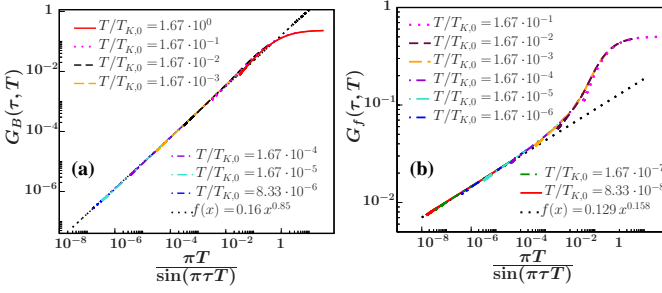


FIG. 3: Scaling of the propagators for the auxiliary boson, $G_B(\tau)$ [panel (a)] and for the pseudo-fermion, $G_f(\tau)$ [panel (b)], for $\epsilon = 0.3$ and the numerical parameters specified in the main text, at the critical coupling $g_c = 25.5T_K^0$.

whose leading behavior is $1/\tau^\epsilon$. Likewise, the three-point correlator is $\sim 1/|\tau_{12}\tau_{13}\tau_{23}|^{\epsilon/2}$, and the four-point correlator $\sum_{i<j} \tau_{ij}^{-\epsilon/3} F(x)$; here the cross-ratio $x = \tau_{12}\tau_{34}/\tau_{13}\tau_{24}$, and $\tau_{ij} \equiv \tau_i - \tau_j$. All these are consistent with the general form of a (boundary) CFT[15].

At finite temperatures we solve equations (11) on real frequencies. The numerical parameters are as in Ref. [9]: We choose $\kappa = 1/2$, $Q/N = 1/2$, and $N_0(\omega) = (1/\pi)\exp(-\omega^2/\pi)$ for the conduction electron density of states. The nominal bare Kondo scale is $T_K^0 N_0(0) \equiv \exp(-1/N_0(0)J_K) \approx 0.02$, for fixed $J_K N_0(0) = 0.8/\pi$. The bosonic bath spectral function $\sum_p \delta(\omega - w_p) \sim \omega^{1-\epsilon}$ is cut off smoothly at $2\omega N_0(0) \approx 0.05$. The imaginary time correlation functions are then obtained from

$$\Phi(\tau) = -\eta \int_{-\infty}^{\infty} d\omega \frac{\exp(-\tau\omega)}{\exp(-\beta\omega) - \eta} \text{Im}(\Phi(\omega + i0^+)), \quad (13)$$

for $0 < \tau \leq \beta$. Here, $\eta = \pm$ for bosonic/fermionic Φ .

Figs. 3(a) and 3(b) show the scaling functions for $\epsilon = 0.3$. For over four (five) decades of $\pi T/\sin(\pi\tau T)$, $G_f(\tau)$ [$G_B(\tau)$] satisfies the conformal form of Eq. (1). (The critical exponents are compatible with the aforementioned analytical results, although correction to scaling is somewhat larger in G_f than in G_B .) Because of their Wick factorizability in terms of $G_f(\tau)$, all the finite-temperature local multi-spin correlation functions will assume the form of a boundary CFT.

Symmetry enhancement at a fixed point is known to happen in other contexts. Moreover, in the case of ordinary (classical) critical points, it is already known that scale invariance is generically accompanied by conformal invariance[15]. What is nontrivial here is that the continuum limit of the bulk part of the Hamiltonian lacks conformal invariance. Our results suggest that, even in this case, the boundary correlators of the boundary QCP can be described in terms of those of an effective model with conformal invariance.

In summary, we have studied the finite-temperature quantum critical properties of the BFKM. Our results suggest that the quantum critical point of the BFKM has

an enhanced symmetry. This insight is expected to be important for the understanding of the underlying field theory of this Kondo-destroying quantum critical point.

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